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                CHEMLIST enhanced with new search and display field
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                JAPIO enhanced with IPC 8 features and functionality
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                 CA/CAplus F-Term thesaurus enhanced
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                 to 50,000
                 CAS REGISTRY updated with new ambiguity codes
        DEC 01
NEWS 9
                 CAS REGISTRY chemical nomenclature enhanced
         DEC 11
NEWS 10
         DEC 14
                 WPIDS/WPINDEX/WPIX manual codes updated
NEWS 11
                GBFULL and FRFULL enhanced with IPC 8 features and
NEWS 12
        DEC 14
                 functionality
                 CA/CAplus pre-1967 chemical substance index entries enhanced
NEWS 13
        DEC 18
                 with preparation role
                 CA/CAplus patent kind codes updated
        DEC 18
NEWS 14
                 MARPAT to CA/CAplus accession number crossover limit increased
        DEC 18
NEWS 15
                 to 50,000
                 MEDLINE updated in preparation for 2007 reload
         DEC 18
NEWS 16
                 CA/CAplus enhanced with more pre-1907 records
NEWS 17 DEC 27
                 CHEMLIST enhanced with New Zealand Inventory of Chemicals
NEWS 18 JAN 08
                 CA/CAplus Company Name Thesaurus enhanced and reloaded
NEWS 19 JAN 16
                 IPC version 2007.01 thesaurus available on STN
NEWS 20 JAN 16
                 WPIDS/WPINDEX/WPIX enhanced with IPC 8 reclassification data
NEWS 21 JAN 16
NEWS 22 JAN 22
                 CA/CAplus updated with revised CAS roles
                 CA/CAplus enhanced with patent applications from India
NEWS 23 JAN 22
                 PHAR reloaded with new search and display fields
NEWS 24
         JAN 29
                 CAS Registry Number crossover limit increased to 300,000 in
NEWS 25
        JAN 29
                 multiple databases
NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT
              MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
              AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.
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FILE 'HOME' ENTERED AT 16:16:32 ON 30 JAN 2007

=> file registry
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

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FILE 'REGISTRY' ENTERED AT 16:16:43 ON 30 JAN 2007 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2007 American Chemical Society (ACS)

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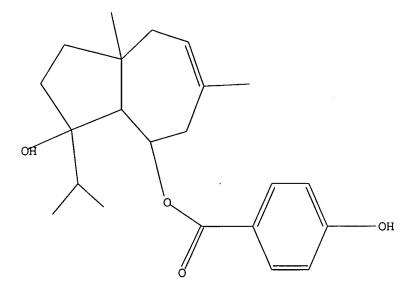
=>
Uploading C:\Program Files\Stnexp\Queries\10 551772 2.str

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 11 sss sam

SAMPLE SEARCH INITIATED 16:17:21 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED -

29 TO ITERATE

100.0% PROCESSED

29 ITERATIONS

4 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLIN

ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

257 TO 903

PROJECTED ANSWERS:

4 TO 200

L2 4 SEA SSS SAM L1

=> d scan

L2 4 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Benzoic acid, 4-hydroxy-3-methoxy-, (3R,3aS,4S,8aS)-1,2,3,3a,4,5,8,8a-octahydro-3-hydroxy-6,8a-dimethyl-3-(1-methylethyl)-8-oxo-4-azulenyl ester (9CI)

MF C23 H30 O6

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L2 4 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Benzoic acid, 4-hydroxy-3-methoxy-, 1,2,3,3a,4,5,8,8a-octahydro-3-hydroxy-

6.8a-dimethyl-3-(1-methylethyl)-4-azulenyl ester (9CI)

MF C23 H32 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 4 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Benzoic acid, 4-hydroxy-, 1,2,3,3a,4,5,8,8a-octahydro-3-hydroxy-6,8adimethyl-3-(1-methylethyl)-1-[(2-methyl-1-oxo-2-butenyl)oxy]-4-azulenyl

ester (9CI)

MF C27 H36 O6

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

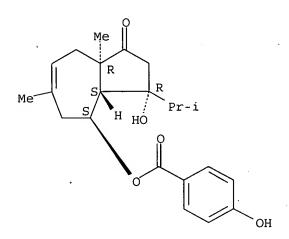
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

L2 4 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Benzoic acid, 4-hydroxy-, (3R,3aS,4S,8aR)-1,2,3,3a,4,5,8,8a-octahydro-3-hydroxy-6,8a-dimethyl-3-(1-methylethyl)-1-oxo-4-azulenyl ester (9CI)

MF C22 H28 O5

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> s l1 sss full FULL SEARCH INITIATED 16:18:04 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 450 TO ITERATE

100.0% PROCESSED 450 ITERATIONS SEARCH TIME: 00.00.01

29 ANSWERS

=> file caplus COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 172.55 172.76

FULL ESTIMATED COST

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=>.s 13/prep

78 L3

4352731 PREP/RL

15 L3/PREP L4

(L3 (L) PREP/RL)

=> d ibib abs hitstr 1-

YOU HAVE REQUESTED DATA FROM 15 ANSWERS - CONTINUE? Y/(N):y

ANSWER 1 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2006:635524 CAPLUS

DOCUMENT NUMBER:

146:19979

TITLE:

Ferutinin stimulates nitric oxide synthase activity in

median eminence of the rat

AUTHOR (S):

Colman-Saizarbitoria, Trina; Boutros, Paulo; Amesty, Angel; Bahsas, Ali; Mathison, Yaira; Garrido, Maria

del Rosario; Israel, Anita

CORPORATE SOURCE:

Laboratory of Bioassays and Natural Products,

Laboratory of Molecular Modeling, School of Pharmacy, Universidad Central de Venezuela, Caracas, Venez. Journal of Ethnopharmacology (2006), 106(3), 327-332

SOURCE:

CODEN: JOETD7; ISSN: 0378-8741

Elsevier B.V. PUBLISHER:

DOCUMENT TYPE: Journal LANGUAGE: English

Several species of Ferula genus have been used in folk medicine in digestive disorders, rheumatism, headache, arthritis, and as tranquilizers, antispasmodic and aphrodisiac. From the dry and powdered roots of Ferula hermonis Boiss was extracted the oxygenated sesquiterpene 1,5-trans-daucane type: ferutinine (1). The structure of (1) was established by spectroscopic methods as: IR, 1H RMN, 13C RMN, COSY, HMBC, HMQC, NOESY, EIMS, and CIMS. The possible signaling pathway of ferutinin

(1) in nervous tissue in vitro was assessed and the results showed that this compound is able to increase nitric oxide synthase activity and inositol monophosphate accumulation (49%, each) in the median eminence of the rat brain, suggesting that compound (1) is associated to the activation of phosphoinositide breakdown and nitric oxide production (NO), the last is a gaseous intercellular messenger known to play a broad role in human biol. from homeostasis to pathol.

41743-44-6P, Ferutinin ΙT

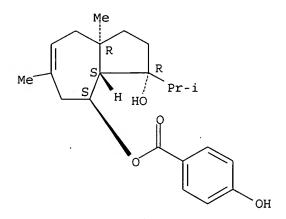
> RL: NPO (Natural product occurrence); PAC (Pharmacological activity); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); USES (Uses)

(ferutinin extracted from Ferula hermonis increased nitric oxide synthase activity, phosphoinositide breakdown and inositol monophosphate accumulation in median eminence rat brain)

RN 41743-44-6 CAPLUS

Benzoic acid, 4-hydroxy-, (3R,3aS,4S,8aR)-1,2,3,3a,4,5,8,8a-octahydro-3-CN hydroxy-6,8a-dimethyl-3-(1-methylethyl)-4-azulenyl ester (9CI) (CA INDEX

Absolute stereochemistry.



REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 2 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN

2005:681613 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 143:302470

Rare trisubstituted sesquiterpenes daucanes from the TITLE:

wild Daucus carota

AUTHOR(S): Ahmed, Ahmed A.; Bishr, Mohktar M.; El-Shanawany,

Mohamed A.; Attia, Eman Z.; Ross, Samir A.; Pare, Paul

Department of Chemistry, Faculty of Science, El-Minia CORPORATE SOURCE:

University, El-Minia, 61519, Egypt

Phytochemistry (Elsevier) (2005), 66(14), 1680-1684 CODEN: PYTCAS; ISSN: 0031-9422 SOURCE:

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal LANGUAGE: English

Phytochem. and biol. investigation of the roots of the wild Daucus carota ssp. carota afforded three new and four known compds., including four sesquiterpenes daucane esters (1-3 [new], and 4), one polyacetylene (5), one sesquiterpene coumarin (6), and sitosterol glucoside. The structures of the new compds. were determined by comprehensive NMR studies, including DEPT, COSY, NOESY, HMQC and HMBC analyses. Based on an agar diffusion assay, 1, 2 and 4-6 were screened and found to contain a range of low antibacterial activities against four gram pos. (Staphylococcus aureus,

Streptomyces scabies, Bacillus subtilis, Bacillus cereus) and two gram neg. species (Pseudomonas aeruginosa, Escherichia coli) as well as antifungal against Fusarium oxysporum and Aspergillus niger using cup agar diffusion assay.

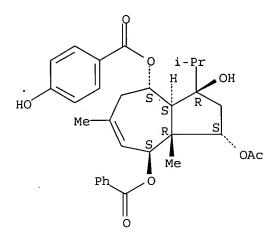
IT 864966-99-4P

RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation) (trisubstituted sesquiterpenes Daucus carota)

RN 864966-99-4 CAPLUS

CN Benzoic acid, 4-hydroxy-, (1R,3S,3aR,4R,8R,8aS)-1-(acetyloxy)-8-(benzoyloxy)-1,2,3,3a,4,5,8,8a-octahydro-3-hydroxy-6,8a-dimethyl-3-(1-methylethyl)-4-azulenyl ester, rel-(+)- (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown. Currently available stereo shown.



REFERENCE COUNT:

THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2004:857419 CAPLUS

DOCUMENT NUMBER:

141:337637

TITLE:

A process for the preparation of ferutinin from Ferula

genus plants

INVENTOR (S):

Bombardelli, Ezio; Fontana, Gabriele; Cristoni, Aldo;

Mercalli, Enrico

PATENT ASSIGNEE(S):

Indena S.P.A., Italy
PCT Int. Appl., 20 pp.

SOURCE:

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND DATE	APPLICATION NO.	DATE
	- -		
WO 2004087179	A1 20041014	WO 2004-EP3055	20040323
W: AE, AG, AL,	AM, AT, AU, AZ,	BA, BB, BG, BR, BW, BY,	BZ, CA, CH,
		DM, DZ, EC, EE, EG, ES,	
		IN, IS, JP, KE, KG, KP,	
		MD, MG, MK, MN, MW, MX,	
		RO, RU, SC, SD, SE, SG,	
		UG, US, UZ, VC, VN, YU,	
		SD, SL, SZ, TZ, UG, ZM,	
		AT, BE, BG, CH, CY, CZ,	

ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG AU 2004-226853 20040323 AU 2004226853 **A**1 20041014 CA 2521100 20041014 CA 2004-2521100 20040323 Α1 EP 1615651 20060118 EP 2004-722572 20040323 Α1 AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, R: IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK BR 2004-9166 20060411 20040323 BR 2004009166 Α 20040323 CN 1767841 Α 20060503 CN 2004-80009111 JP 2006522043 T 20060928 -JP 2006-504815 20040323 NO 2005004545 Α 20051006 NO 2005-4545 20051003 US 2006275246 A1 20061207 US 2005-551772 20051003 IT 2003-MI661 20030404 PRIORITY APPLN. INFO.: Α WO 2004-EP3055 W 20040323

AB The invention relates to a process for the preparation of ferutinin from Ferula spp exts. comprising basic hydrolysis of the exts. and treatment with p-pivaloyloxybenzoic acid. The invention relates also to the use of the exts. and ferutinin in the cosmetic and dermatol. field.

IT 41743-44-6P, Ferutinin

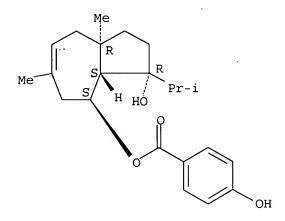
RL: BPN (Biosynthetic preparation); COS (Cosmetic use); NPO (Natural product occurrence); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); USES (Uses)

(process for the preparation of ferutinin from Ferula genus plants)

RN 41743-44-6 CAPLUS

CN Benzoic acid, 4-hydroxy-, (3R,3aS,4S,8aR)-1,2,3,3a,4,5,8,8a-octahydro-3-hydroxy-6,8a-dimethyl-3-(1-methylethyl)-4-azulenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2004:690919 CAPLUS

DOCUMENT NUMBER:

141:366336

TITLE:

Structure-Activity Relationships of the Estrogenic Sesquiterpene Ester Ferutinin. Modification of the

Terpenoid Core

AUTHOR(S):

Appendino, Giovanni; Spagliardi, Paola; Sterner, Olov;

Milligan, Stuart

CORPORATE SOURCE:

Dipartimento di Scienze Chimiche Alimentari Farmaceutiche e Farmacologiche, Universita del

Piemonte Orientale, Novara, 28100, Italy

SOURCE:

Journal of Natural Products (2004), 67(9), 1557-1564

CODEN: JNPRDF; ISSN: 0163-3864

American Chemical Society

Journal English

OTHER SOURCE(S):

PUBLISHER: DOCUMENT TYPE:

LANGUAGE:

CASREACT 141:366336

GT

Esterification of p-hydroxybenzoic acid, a very weak estrogenic compound, AB with the daucane alc. jaeschkeanadiol (I; R = H) leads to a spectacular magnification of the estrogenic activity. To identify the structural elements responsible for this effect, the terpenoid core of jaeschkeanadiol p-hydroxybenzoate (ferutinin, I; R = COC6H4OH-4) was modified, capitalizing on the presence of two functionalities, the monoacylated, hydrogen-bonded 1,3-diol system and the double bond. hydrogen bonding, while possibly useful, was not critical for activity, while hydrogenation and cyclopropanation of the double bond were tolerated. Conversely, oxidative modifications of the double bond that placed a hydroxyl on the α -face of the mol. proved detrimental. Taken together, these observations identified the substitution at C-8/C-9 as critical for activity.

109517-73-9P, 14-Hydroxyferutinin 302342-52-5P, ΙT

14-Oxoferutinin

RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and estrogenic activity of ferutinin analogs)

109517-73-9 CAPLUS RN

Benzoic acid, 4-hydroxy-, (3R,3aS,4S,8aR)-1,2,3,3a,4,5,8,8a-octahydro-3-CN hydroxy-6-(hydroxymethyl)-8a-methyl-3-(1-methylethyl)-4-azulenyl ester, rel-(+)- (9CI) (CA INDEX NAME)

.Rotation (+). Absolute stereochemistry unknown.

302342-52-5 CAPLUS RN

Benzoic acid, 4-hydroxy-, (3R,3aS,4S,8aR)-6-formyl-1,2,3,3a,4,5,8,8a-CN octahydro-3-hydroxy-8a-methyl-3-(1-methylethyl)-4-azulenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

REFERENCE COUNT:

THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS 26

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

CAPLUS COPYRIGHT 2007 ACS on STN L4ANSWER 5 OF 15

ACCESSION NUMBER: 2004:541439 CAPLUS

DOCUMENT NUMBER: 141:346209

TITLE: Structure of Samferine

Eshbakova, K. A.; Saidkhodzhaev, A. I. AUTHOR (S):

S. Yu. Yunusov Institute of the Chemistry of Plant CORPORATE SOURCE:

Substances, Academy of Sciences of the Republic of

Uzbekistan, Uzbekistan

SOURCE: Chemistry of Natural Compounds (Translation of Khimiya

Prirodnykh Soedinenii) (2004), 40(2), 194-195

II

CODEN: CHNCA8; ISSN: 0009-3130

Kluwer Academic/Consultants Bureau PUBLISHER:

Journal DOCUMENT TYPE:

English LANGUAGE:

GI

AB The authors have isolated a new compound samferine (I), of formula C22H30O5, from the roots of F. samarcandica Korov. Alkaline hydrolysis of I produced a sesquiterpene alc. samferol (II), of the formula C15H26O3, from the neutral part of the hydrolyzate.

IT 774577-57-0P, Samferine

Ι

RL: NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); RCT (Reactant); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); RACT (Reactant or reagent)

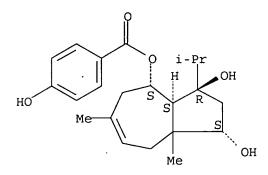
(isolation and mol. structure of sesquiterpene ester samferine from F.

samarcandica)

774577-57-0 CAPLUS RN

Benzoic acid, 4-hydroxy-, (1R,3S,3aR,4R)-1,2,3,3a,4,5,8,8a-octahydro-1,3-CN dihydroxy-6,8a-dimethyl-3-(1-methylethyl)-4-azulenyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry. Currently available stereo shown.



REFERENCE COUNT:

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

CAPLUS COPYRIGHT 2007 ACS on STN ANSWER 6 OF 15

6

ACCESSION NUMBER:

2002:709827 CAPLUS

DOCUMENT NUMBER:

137:363261

TITLE: AUTHOR (S): Daucane phytoestrogens: a structure-activity study Appendino, Giovanni; Spagliardi, Paola; Cravotto, Giancarlo; Pocock, Victoria; Milligan, Stuart

CORPORATE SOURCE:

Dipartimento di Scienze Chimiche, Alimentari,

Farmaceutiche e Farmacologiche, Universita del Piemonte Orientale, Novara, 28100, Italy

SOURCE:

Journal of Natural Products (2002), 65(11), 1612-1615

CODEN: JNPRDF; ISSN: 0163-3864

PUBLISHER:

American Chemical Society

DOCUMENT TYPE:

Journal

LANGUAGE:

English

The estrogenic activity of a series of analogs of the daucane ester ferutinin modified at the acyl moiety was investigated in a yeast screen containing the human estrogen receptor α . Rather strict structure-activity relationships were observed Thus, while the parent polyol (jaeschkeanadiol) was inactive, the presence of a p-hydroxybenzoyl moiety was necessary for activity in the yeast screen. Homologation and vinylation were both detrimental for activity, as were methylation of the p-hydroxyl substituent and the introduction of oxygen functions on the adjacent carbons.

41743-44-6DP, Ferutinin, derivs. 41743-44-6P, Ferutinin IT 54526-95-3P 126783-56-0P

RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(daucane phytoestrogens: a structure-activity study)

41743-44-6 CAPLUS RN

CN Benzoic acid, 4-hydroxy-, (3R,3aS,4S,8aR)-1,2,3,3a,4,5,8,8a-octahydro-3hydroxy-6,8a-dimethyl-3-(1-methylethyl)-4-azulenyl ester (9CI) (CA INDEX NAME)

RN 41743-44-6 CAPLUS

CN Benzoic acid, 4-hydroxy-, (3R,3aS,4S,8aR)-1,2,3,3a,4,5,8,8a-octahydro-3-hydroxy-6,8a-dimethyl-3-(1-methylethyl)-4-azulenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 54526-95-3 CAPLUS

CN Benzoic acid, 4-hydroxy-3-methoxy-, (3R,3aS,4S,8aR)-1,2,3,3a,4,5,8,8a-octahydro-3-hydroxy-6,8a-dimethyl-3-(1-methylethyl)-4-azulenyl ester (9CI) (CA INDEX NAME)

RN 126783-56-0 CAPLUS

CN Benzoic acid, 3,4-dihydroxy-, (3R,3aS,4S,8aR)-1,2,3,3a,4,5,8,8a-octahydro-3-hydroxy-6,8a-dimethyl-3-(1-methylethyl)-4-azulenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:315620 CAPLUS

DOCUMENT NUMBER: 137:332761

TITLE: Antimicrobial sesquiterpene from the roots of Ferula

harmonis

AUTHOR(S): Al-Sha'er, M.; Darwish, R. M.; Aburjai, T.

CORPORATE SOURCE: Department of Pharmaceutical Sciences, Faculty of

Pharmacy, University of Jordan, Amman, 11942, Jordan

SOURCE: Acta Technologiae et Legis Medicamenti (2001), 12(3),

255-264

CODEN: ATLMEQ; ISSN: 1121-2098

PUBLISHER: Maccari Editore

DOCUMENT TYPE: Journal LANGUAGE: English

AB Two known sesquiterpenes were isolated for the first time from the roots of Ferula harmonis F. (Umbelliferae). Their structures were assigned by spectroscopic (MS, 1H-NMR, 13C-NMR) and phys. means as ferutinin and teferidine. The antimicrobial activity of the crude exts. and the isolated compds. was tested against four different microorganisms. Ferutinin showed good antibacterial activity against S. aureus and weak antifungal activity against A. niger. Teferidine, showed no antimicrobial activity against the tested microorganisms. Our results revealed the importance of the phenolic hydroxyl group for the antimicrobial activity of these compds.

IT 41743-44-6P, Ferutinin

RL: NPO (Natural product occurrence); PAC (Pharmacological activity); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological actudy); OCCU (Occurrence); PREP (Preparation); USES (Uses)

study); OCCU (Occurrence); PREP (Preparation); USES (Uses) (antimicrobial sesquiterpene from the roots of Ferula harmonis)

RN 41743-44-6 CAPLUS

CN Benzoic acid, 4-hydroxy-, (3R,3aS,4S,8aR)-1,2,3,3a,4,5,8,8a-octahydro-3-hydroxy-6,8a-dimethyl-3-(1-methylethyl)-4-azulenyl ester (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS 17 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

CAPLUS COPYRIGHT 2007 ACS on STN ANSWER 8 OF 15

ACCESSION NUMBER:

2001:771413 CAPLUS

DOCUMENT NUMBER:

136:180636

TITLE:

Sesquiterpenoids from the fruits of Ferula kuhistanica

and antibacterial activity of the constituents of F.

AUTHOR (S):

Tamemoto, Kimiko; Takaishi, Yoshihisa; Chen, Bei; Kawazoe, Kazuyoshi; Shibata, Hirofumi; Higuti,

Tomihiko; Honda, Gisho; Ito, Michiho; Takeda, Yoshio;

Kodzhimatov, Olimjon K.; Ashurmetov, Ozodbek

CORPORATE SOURCE:

Faculty of Pharmaceutical Sciences, University of

Tokushima, Tokushima, 770-8505, Japan Phytochemistry (2001), 58(5), 763-767 CODEN: PYTCAS; ISSN: 0031-9422

PUBLISHER:

SOURCE:

Elsevier Science Ltd.

DOCUMENT TYPE:

Journal English

LANGUAGE: GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Et acetate exts. of the air-dried fruits of Ferula kuhistanica afforded AB three daucane esters: kuhistanicaols H, I and J (I, II, and III, resp.), together with nine other known compds. Their structures were established on the basis of spectroscopic evidence. Isolated compds. in this paper and previously reported compds. from the roots and stems of F. kuhistanica were tested for antibacterial activity. Some of them were selectively toxic against Gram-pos. bacteria, including methicillin-sensitive and methicillin-resistant Staphylococcus aureus (MSSA and MRSA).

IT 41743-44-6P

RL: PAC (Pharmacological activity); PRP (Properties); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(purification from Ferula kuhistanica fruit and antibacterial activity of)

41743-44-6 CAPLUS RN

Benzoic acid, 4-hydroxy-, (3R,3aS,4S,8aR)-1,2,3,3a,4,5,8,8a-octahydro-3-CN hydroxy-6,8a-dimethyl-3-(1-methylethyl)-4-azulenyl ester (9CI) (CA INDEX NAME)

IT 54526-95-3P

RL: PAC (Pharmacological activity); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(purification from Ferula kuhistanica fruit and antibacterial activity of)

RN 54526-95-3 CAPLUS

CN Benzoic acid, 4-hydroxy-3-methoxy-, (3R,3aS,4S,8aR)-1,2,3,3a,4,5,8,8a-octahydro-3-hydroxy-6,8a-dimethyl-3-(1-methylethyl)-4-azulenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 399035-10-0P, Kuhistanicaol I

RL: NPO (Natural product occurrence); PAC (Pharmacological activity); PRP (Properties); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); USES (Uses)

(sesquiterpenoids from the fruit of Ferula kuhistanica and antibacterial activity of the constituents of F. kuhistanica)

RN 399035-10-0 CAPLUS

CN Benzoic acid, 4-hydroxy-3-methoxy-, (3R,3aS,4S,8R,8aS)-1,2,3,3a,4,5,8,8a-octahydro-3,8-dihydroxy-6,8a-dimethyl-3-(1-methylethyl)-1-oxo-4-azulenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

REFERENCE COUNT:

14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

CORPORATE SOURCE:

2001:286907 CAPLUS

DOCUMENT NUMBER:

135:43518

TITLE:

Daucane aryl esters composition from the Lebanese

Ferula hermonis Boiss. (zallooh root)

AUTHOR (S):

Diab, Youssef; Dolmazon, Rene; Bessiere, Jean-Marie Universite Libanaise, Faculte des Sciences-2, Jdaidet

el-Matn, Lebanon

SOURCE:

Flavour and Fragrance Journal (2001), 16(2), 120-122

CODEN: FFJOED; ISSN: 0882-5734

PUBLISHER:

John Wiley & Sons Ltd.

DOCUMENT TYPE:

Journal

LANGUAGE:

English

The dichloromethane extract of Ferula hermonis roots, isolated in 26.5% yield based on dry roots, contained as principal components p-hydroxybenzoate and benzoate of jaeschkeanadiol (52% and 30%, resp.). Some other aryl esters of jaeschkeanadiol and 2,3-epoxide jaeschkeanadiol, as well as $\alpha\text{-bisabolol},$ were present in small amts.

IT 41743-44-6P, Jaeschkeanadiol p-hydroxybenzoate 54526-95-3P
, Teferin

RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study);

OCCU (Occurrence); PREP (Preparation)
(daucane aryl esters composition from the Lebanese Ferula hermonis (zallooh root))

RN 41743-44-6 CAPLUS

CN Benzoic acid, 4-hydroxy-, (3R,3aS,4S,8aR)-1,2,3,3a,4,5,8,8a-octahydro-3-hydroxy-6,8a-dimethyl-3-(1-methylethyl)-4-azulenyl ester (9CI) (CA INDEX NAME)

RN 54526-95-3 CAPLUS

CN Benzoic acid, 4-hydroxy-3-methoxy-, (3R,3aS,4S,8aR)-1,2,3,3a,4,5,8,8a-octahydro-3-hydroxy-6,8a-dimethyl-3-(1-methylethyl)-4-azulenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN

18

ACCESSION NUMBER:

2001:4915 CAPLUS

DOCUMENT NUMBER:

134:219768

TITLE:

Sesquiterpenes from Ferula hermonis Boiss

Galal, A.

CORPORATE SOURCE:

National Center for Natural Products Research, School of Pharmacy, University of Mississippi, University,

MS, 38677, USA

SOURCE:

Pharmazie (2000), 55(12), 961-962 CODEN: PHARAT; ISSN: 0031-7144

PUBLISHER:

AUTHOR (S):

Govi-Verlag Pharmazeutischer Verlag

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB The roots of Ferula hermonis yielded the new 8,9-epoxy derivative of the carotane sesquiterpene jaeschkeanadiol, together with 2 other known sesquiterpenes: (+)- α -bisabolol and jaeschkeanadiol vanillate. The identities of the isolated compds. were established from their spectral data and by comparison with published reports.

IT 54526-95-3P

RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)

(sesquiterpenes from Ferula hermonis)

RN 54526-95-3 CAPLUS

CN Benzoic acid, 4-hydroxy-3-methoxy-, (3R,3aS,4S,8aR)-1,2,3,3a,4,5,8,8a-octahydro-3-hydroxy-6,8a-dimethyl-3-(1-methylethyl)-4-azulenyl ester (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 11 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN

9

ACCESSION NUMBER:

2000:590836 CAPLUS

DOCUMENT NUMBER:

133:319520

TITLE:

Sesquiterpenoids from Ferula kuhistanica

AUTHOR (S):

Chen, B.; Teranishi, R.; Kawazoe, K.; Takaishi, Y.; Honda, G.; Itoh, M.; Takeda, Y.; Kodzhimatov, O. K.

CORPORATE SOURCE:

Fac. Pharm. Sci., Univ. Tokushima, Tokushima,

770-8505, Japan

SOURCE:

Phytochemistry (2000), 54(7), 717-722 CODEN: PYTCAS; ISSN: 0031-9422

PUBLISHER:

Elsevier Science Ltd.

DOCUMENT TYPE:

Journal

LANGUAGE:

English

GI

Methanol exts. of the air-dried roots and stems of Ferula kuhistanica AB afforded seven daucane-type sesquiterpenes, called kuhistanicaol A-G (e.g. I, kuhistanicaol A) together with 13 known daucane esters. Their structures were established on the basis of spectroscopic evidence and the results of chemical reactions.

302342-52-5P, Kuhistanicaol B 302342-54-7P, ΙT

Kuhistanicaol D

RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)

(from Ferula kuhistanica)

302342-52-5 CAPLUS RN

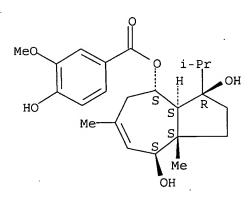
Benzoic acid, 4-hydroxy-, (3R,3aS,4S,8aR)-6-formyl-1,2,3,3a,4,5,8,8a-CN octahydro-3-hydroxy-8a-methyl-3-(1-methylethyl)-4-azulenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 302342-54-7 CAPLUS

CN Benzoic acid, 4-hydroxy-3-methoxy-, (3R,3aS,4S,8S,8aS)-1,2,3,3a,4,5,8,8a-octahydro-3,8-dihydroxy-6,8a-dimethyl-3-(1-methylethyl)-4-azulenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 12 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1999:294524 CAPLUS

Correction of: 1998:104683

DOCUMENT NUMBER: 130:294014

Correction of: 128:203022

TITLE: Chemical constituents of rocks of Ferula licentiana

var. tunshanica and F. kingdonwardii and their

systematical significance

AUTHOR(S): Wang, Nianhe; Yuan, Changqi; Baba, Kimie; Taniguchi,

Masahiko; Doi, Mitsunobu

CORPORATE SOURCE: Institute of Botany, Jiangsu Province and Chinese

Academy of Sciences, Nanjing, 210014, Peop. Rep. China

SOURCE: Zhiwu Ziyuan Yu Huanjing (1997), 6(4), 15-18, 49

CODEN: ZZYHEJ; ISSN: 1004-0978

PUBLISHER: Zhiwu Ziyuan Yu Huanjing Bianjibu

DOCUMENT TYPE: Journal LANGUAGE: Chinese

AB Latifolone, p-anisic acid, veratric acid, fercomin, ferutidin, ferutinin, jaeschkeanadiol varatrate, terferin, 1-(7,8-dimethoxy-5,6-methylenedioxy phenyl)propyl (Z)-2-methyl-1-butenoate and 4,11,11,10-tetramethyl-1,10-oxirane-4-ene-6-germacrane varatrate were isolated from the ether exts. of the roots of Ferula licentiana Hand.-Mazz. var. tunshanica Shan et Q. X. Liu and F. kingdonwardii Wolff. Among them, 1-(7,8-dimethoxy-5,6-

methylenedioxy phenyl) Pr (Z)-2-methyl-butenoate is a new compound These two Ferulious plants were distributed on the border of the distribution of this genus, but 7-0-sesquiterpene, one of the characteristic compds. Of this genus, was not detectable in these species, and the components of these two plants were similar and comparatively simple. It was suggested that perhaps Ferula L., like some other Umbelliferous plants such as Angelica L., also originated from the south-west China.

41743-44-6P, Ferutinin 54526-95-3P, Teferin

RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)

(chemical constituents of roots of ferula licentiana var. tunshanica and F. kingdonwardii and systematical significance)

RN 41743-44-6 CAPLUS

IT

CN Benzoic acid, 4-hydroxy-, (3R,3aS,4S,8aR)-1,2,3,3a,4,5,8,8a-octahydro-3-hydroxy-6,8a-dimethyl-3-(1-methylethyl)-4-azulenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 54526-95-3 CAPLUS

CN Benzoic acid, 4-hydroxy-3-methoxy-, (3R,3aS,4S,8aR)-1,2,3,3a,4,5,8,8aoctahydro-3-hydroxy-6,8a-dimethyl-3-(1-methylethyl)-4-azulenyl ester (9CI) (CA INDEX NAME)

ACCESSION NUMBER: 1998:104683 CAPLUS

DOCUMENT NUMBER: 128:203022

TITLE: Chemical constituents of roots of Ferula licentiana

var. tunshanica and F. kingdonwardii and their

systematical significance

AUTHOR(S): Wang, Nianhe; Yuan, Changqi; Kimie Baba; Masahiko

Taniguch; Mitsunobu Doi

CORPORATE SOURCE: Institute of Botany, Jiangsu Province and Chinese

Academy of Sciences, Nanjing, 210014, Peop. Rep. China

SOURCE: Zhiwu Ziyuan Yu Huanjing (1997), 6(4), 15-18, 49

CODEN: ZZYHEJ; ISSN: 1004-0978

Zhiwu Ziyuan Yu Huanjing Bianjibu

DOCUMENT TYPE: Journal LANGUAGE: Chinese

PUBLISHER:

Latifolone, p-anisic acid, veratric acid, fercomin, ferutidin, ferutinin, jaeschkeanadiol varatrate, terferin, 1-(7,8- dimethoxy-5,6-methylenedioxy phenyl)propyl (Z)-2-methyl-1-butenoate and 4,11,11,10-tetramethyl-1,10-oxirane-4-ene-6-germacrane varatrate were isolated from the ether exts. Of the roots of Ferula licentiana Hand.-Mazz. var. tunshanica Shan et Q. X. Liu and F. kingdonwardii Wolff. Among them, 1-(7,8-dimethoxy-5,6-methylenedioxy phenyl) Pr (Z)-2-methyl-butenoate is a new compound These two Ferulious plants were distributed on the border of the distribution of this genus, but 7-O-sesquiterpene, one of the characteristic compds. of this genus, was not detectable in these species, and the components of these two plants were similar and comparatively simple. It was suggested that perhaps Ferula L., like some other Umbelliferous plants such as Angelica L., also originated from the south-west China.

IT 41743-44-6P, Ferutinin 54526-95-3P, Teferin RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study);

OCCU (Occurrence); PREP (Preparation)
(chemical constituents of roots of ferula licentiana var. tunshanica and F. kingdonwardii and systematical significance)

RN 41743-44-6 CAPLUS

CN Benzoic acid, 4-hydroxy-, (3R,3aS,4S,8aR)-1,2,3,3a,4,5,8,8a-octahydro-3-hydroxy-6,8a-dimethyl-3-(1-methylethyl)-4-azulenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 54526-95-3 CAPLUS

CN Benzoic acid, 4-hydroxy-3-methoxy-, (3R,3aS,4S,8aR)-1,2,3,3a,4,5,8,8a-octahydro-3-hydroxy-6,8a-dimethyl-3-(1-methylethyl)-4-azulenyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1995:844841 CAPLUS

DOCUMENT NUMBER: 124:4913

TITLE: Carotane sesquiterpenes from Ferula sinaica Boiss

growing in Egypt

AUTHOR(S): Ibraheim, Zidan Z.; Darwish, Faten M. M.; Abdel-Halim,

Osama B.; Halim, Ahmed F.

CORPORATE SOURCE: Faculty Pharmacy, Assiut University, Assiut, Egypt

SOURCE: Alexandria Journal of Pharmaceutical Sciences (1995),

9(2), 115-20

CODEN: AJPSES; ISSN: 1110-1792

PUBLISHER: University of Alexandria, Faculty of Pharmacy

DOCUMENT TYPE: Journal LANGUAGE: English

AB Phytochem. investigation of the air-dried roots of Ferula sinaica Boiss

resulted in the isolation and identification of ten known carotane

sesquiterpenes. Of these, seven compds. were isolated for the first time

from this species and characterized as: $1-\alpha$ -angeloyloxy- $5-\alpha$ -p-

methoxybenzoyloxy- $10-\beta$ -hydroxydauc-2-ene, lancerodiol

p-methoxybenzoate, p-methoxybenzoate of epoxyjaeschkeanadiol,

p-hydroxybenzoate of epoxyjaeschkeanadiol, isolancerotriol-5-p-

methoxybenzoate, $1\alpha-\beta$ -hydroxy-5- α -p-methoxybenzoyloxy-10-

 β -hydroxydauc-2-ene and 1- α -hydroxy-5- α -p-

methoxybenzoyloxy-10- β -hydroxydauc-2-ene in addition to

 β -sitosterol. Identification of the isolated compds. was established using phys. and spectroscopic methods.

IT 41743-44-6P 119425-93-3P 170971-43-4P,

Ferulinkiol $1-\alpha$ -hydroxy- $5-\alpha$ -p-hydroxybenzoate

RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)

(carotane sesquiterpenes from Ferula sinaica growing in Egypt)

RN 41743-44-6 CAPLUS

CN Benzoic acid, 4-hydroxy-, (3R,3aS,4S,8aR)-1,2,3,3a,4,5,8,8a-octahydro-3-hydroxy-6,8a-dimethyl-3-(1-methylethyl)-4-azulenyl ester (9CI) (CA INDEX NAME)

RN 119425-93-3 CAPLUS

CN Benzoic acid, 4-hydroxy-, 1,2,3,3a,4,5,8,8a-octahydro-3-hydroxy-6,8a-dimethyl-3-(1-methylethyl)-8-[(2-methyl-1-oxo-2-butenyl)oxy]-4-azulenyl ester, [3R-[3 α ,3a β ,4 β ,8 β (Z),8a α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 170971-43-4 CAPLUS

CN Benzoic acid, 4-hydroxy-, 1,2,3,3a,4,5,8,8a-octahydro-3,8-dihydroxy-6,8a-dimethyl-3-(1-methylethyl)-4-azulenyl ester, (3α,3aβ,4β,8.
beta:,8aα)- (9CI) (CA INDEX NAME)

Relative stereochemistry. Currently available stereo shown.

ANSWER 15 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1980:471992 CAPLUS

DOCUMENT NUMBER:

93:71992

TITLE:

Structure of jaeschferin

AUTHOR(S):

Bizhanova, K. B.; Saidkhodzhaev, A. I.; Malikov, V. M.

CORPORATE SOURCE:

Inst. Khim. Rastit. Veshchestv, Tashkent, USSR

SOURCE:

Khimiya Prirodnykh Soedinenii (1980), (1), 127-8

CODEN: KPSUAR; ISSN: 0023-1150

DOCUMENT TYPE:

Journal

LANGUAGE:

Russian

GI

$$\begin{array}{c|c} \text{OH} & \text{Me} \\ \hline \text{Me} & \text{OMe} \\ \\ \text{H} & \text{O}_2\text{C} & \text{OH} \\ \\ \text{CHMe}_2 & \text{O}_2\text{C} & \text{I} \end{array}$$

The structure of jaeschferin (I), a sesquiterpene ester isolated from AB Ferula iaeschkeana, was confirmed by mass and NMR spectra.

IT 74345-97-4P

> RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

74345-97-4 CAPLUS RN

Benzoic acid, 4-hydroxy-3-methoxy-, 1,2,3,3a,4,5,8,8a-octahydro-1,3-CN dihydroxy-6,8a-dimethyl-3-(1-methylethyl)-4-azulenyl ester, diacetate, $(1\alpha, 3\alpha, 3a\beta, 4\beta, 8a\alpha)$ - (9CI) (CA INDEX NAME)

CM 1

74285-96-4 CRN

CMF C23 H32 O6

Rotation (+). Absolute stereochemistry unknown.

CM 2

CRN 64-19-7 CMF C2 H4 O2

=> d his

(FILE 'HOME' ENTERED AT 16:16:32 ON 30 JAN 2007)

FILE 'REGISTRY' ENTERED AT 16:16:43 ON 30 JAN 2007

L1 STRUCTURE UPLOADED

L2 4 S L1 SSS SAM

L3 29 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 16:18:12 ON 30 JAN 2007

L4 15 S L3/PREP

=>